

Title: Time Evolution in Time-Dependent Systems

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In time-independent systems, time-evolution is remarkably simple. The unitary operator is:

$$\hat{U}(t_0 + \delta t, t_0) = e^{-\frac{i\hat{H}\delta t}{\hbar}} \quad (1)$$

In time-dependent systems, there is enhanced complication:

$$\hat{U}(t_0 + \delta t, t_0) = e^{-\frac{i \int_{t_0}^{t_0+\delta t} dt \hat{H}(t)}{\hbar}} \quad (2)$$

Though the time-dependent Hamiltonian must then be considered as an integral, the critical step in evaluating time evolution is to consider the time-independent case as an exact instantaneous solution, such that that exact time evolution in the system comes from evaluating the infinite product of the instantaneous exponential Hamiltonians. Then, we attain the following formula:

$$\begin{aligned} \hat{U}(t, t_0) &= \lim_{N \rightarrow \infty} \prod_{k=0}^N e^{-\frac{i\hat{H}(t_k)\delta t}{\hbar}} \\ &= \lim_{N \rightarrow \infty} e^{-\frac{i\hat{H}(t_N)\delta t}{\hbar}} e^{-\frac{i\hat{H}(t_{N-1})\delta t}{\hbar}} \dots e^{-\frac{i\hat{H}(t_1)\delta t}{\hbar}} e^{-\frac{i\hat{H}(t_0)\delta t}{\hbar}} \end{aligned} \quad (3)$$

where $\delta t = \lim_{N \rightarrow \infty} \frac{t-t_0}{N}$. Notice the time ordering on the left side to the right side. This is an important aspect of the formulation since the Hamiltonians at different times do not commute with one another. However, what we do know is that the exponential argument (with the infinitesimal δt) is very small, and thus can be expanded into the following sequence of products:

$$\begin{aligned} \hat{U}(t, t_0) &= \lim_{N \rightarrow \infty} \prod_{k=0}^N \left(1 - \frac{i\hat{H}(t_k)\delta t}{\hbar} \right) \\ &= \lim_{N \rightarrow \infty} \left(1 - \frac{i\hat{H}(t_N)\delta t}{\hbar} \right) \dots \left(1 - \frac{i\hat{H}(t_1)\delta t}{\hbar} \right) \left(1 - \frac{i\hat{H}(t_0)\delta t}{\hbar} \right) \\ &= \lim_{N \rightarrow \infty} \left(1 - \left(\frac{i}{\hbar} \right) \sum_{k=0}^N \hat{H}(t_k) \delta t + \left(\frac{i}{\hbar} \right)^2 \sum_{k=1}^N \sum_{j=0}^{k-1} \hat{H}(t_k) \hat{H}(t_j) (\delta t)^2 - \dots \right) \\ &= 1 + \lim_{N \rightarrow \infty} \sum_{k=1}^N \left(\frac{-i}{\hbar} \right)^k \int_{t_0}^t dt_k \hat{H}(t_k) \prod_{\ell=0}^{k-2} \int_{t_0}^{t_{\ell+2}} dt_{\ell+1} \hat{H}(t_{\ell+1}) \end{aligned} \quad (4)$$

where note that the upper bound of each integral is the integration variable of the next leftward integral. This corresponds to the time ordering and non-commutativity of Hamiltonian at different

times, where $t_\ell > t_{\ell-1}$, and the product is a left product (i.e. the next term left multiplies the previous term). Formally, this last line corresponds to what is known as the Dyson Series.

However, for this post, I am going to take a different approach - one which shines light on the subtleties of Equation 3. To consider an example, consider 1D Quantum Harmonic Oscillator with time dependent frequency $\omega(t)$. In the last post, we showed the following:

$$\begin{aligned}\Phi_{mn}(t) &= \langle \psi_m(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle = -\frac{1}{4} \frac{\sqrt{(n+1)_2}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} \delta_{(n+2),m} + \frac{1}{4} \frac{\sqrt{(n-1)_2}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} \delta_{(n-2),m} \\ |\psi_n(x, t)\rangle &= \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega(t)}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega(t)x^2}{2\hbar}} H_n \left(\sqrt{\frac{m\omega(t)}{\hbar}} x \right) \\ E_n(t) &= \hbar \left(n + \frac{1}{2} \right) \omega(t), \quad \frac{\partial E_n(t)}{\partial t} = \hbar \left(n + \frac{1}{2} \right) \frac{\partial \omega(t)}{\partial t} \\ \hat{H}(t) &= \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2(t) x^2 \\ \frac{\partial \hat{H}(t)}{\partial t} &= \begin{bmatrix} \frac{\partial E_0(t)}{\partial t} & 0 & 2\hbar\omega(t)\Phi_{02}(t) & \dots \\ 0 & \frac{\partial E_1(t)}{\partial t} & 0 & \dots \\ -2\hbar\omega(t)\Phi_{20}(t) & 0 & \frac{\partial E_2(t)}{\partial t} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}\end{aligned}$$

In this example, all $\Phi_{mn}(t) = 0$ except $\Phi_{n+2,n}(t)$ and $\Phi_{n-2,n}(t)$, and the diagonal elements of $\frac{\partial \hat{H}(t)}{\partial t}$ are determined by Hellmann-Feynman theorem. From this mathematics, we can carry out the following calculation on Equation 3. Assume that the state vector starts in the ground state at $t = 0$ (that is, $|\Psi(x, 0)\rangle = |\psi_0(x, 0)\rangle$). Then, the time evolution calculation can be carried out as follows (with $\delta t = \frac{t}{N}$):

$$\begin{aligned}\hat{U}(t, 0) |\Psi(x, 0)\rangle &= \lim_{N \rightarrow \infty} \prod_{k=0}^N e^{-\frac{i\hat{H}(t_k)\delta t}{\hbar}} |\psi_0(x, 0)\rangle \\ &= \lim_{N \rightarrow \infty} e^{-\frac{i\hat{H}(t)\delta t}{\hbar}} e^{-\frac{i\hat{H}(t-\delta t)\delta t}{\hbar}} \dots e^{-\frac{i\hat{H}(\delta t)\delta t}{\hbar}} e^{-\frac{i\hat{H}(0)\delta t}{\hbar}} |\psi_0(x, 0)\rangle \\ &= \lim_{N \rightarrow \infty} \dots e^{-\frac{i\hat{H}(2\delta t)\delta t}{\hbar}} e^{-\frac{i\hat{H}(\delta t)\delta t}{\hbar}} \sum_{m_0=0}^{\infty} |\psi_{m_0}(x, \delta t)\rangle \langle \psi_{m_0}(x, \delta t) | e^{-\frac{i\hat{H}(0)\delta t}{\hbar}} |\psi_0(x, 0)\rangle \\ &= \lim_{N \rightarrow \infty} \dots e^{-\frac{i\hat{H}(2\delta t)(2\delta t)\delta t}{\hbar}} \left(\sum_{m_0=0}^{\infty} e^{-\frac{iE_{m_0}(\delta t)\delta t}{\hbar}} |\psi_{m_0}(x, \delta t)\rangle \left(\langle \psi_{m_0}(x, 0) | + \frac{\partial \langle \psi_{m_0}(x, 0) |}{\partial t} \delta t \right) e^{-\frac{iE_0(0)\delta t}{\hbar}} |\psi_0(x, 0)\rangle \right) \\ &= \lim_{N \rightarrow \infty} \dots e^{-\frac{i\hat{H}(2\delta t)\delta t}{\hbar}} \left(e^{-\frac{iE_0(\delta t)\delta t}{\hbar}} e^{-\frac{iE_0(0)\delta t}{\hbar}} |\psi_0(x, \delta t)\rangle - e^{-\frac{iE_2(\delta t)\delta t}{\hbar}} e^{-\frac{iE_0(0)\delta t}{\hbar}} \Phi_{20}(\delta t) |\psi_2(x, \delta t)\rangle \delta t \right)\end{aligned}\tag{5}$$

And just from this preliminary calculation, one can observe some important structure in the complete calculation. For one, the time evolved state vector will be composed of only linear combinations of the even energy eigenstates with the product of their energy eigenvalue phase factors. One can imagine the following time evolution term for the state vector that has no mixing

from the other eigenstate states.

$$\begin{aligned}
U_0(t, 0) |\Psi(x, 0)\rangle &= \lim_{N \rightarrow \infty} e^{-\frac{i\delta t}{\hbar} \sum_{n=0}^N E_0(\frac{n}{N}t)} |\psi_0(x, t)\rangle \\
&= \lim_{N \rightarrow \infty} e^{-\frac{it}{\hbar} \frac{1}{N} \sum_{n=0}^N E_0(\frac{n}{N}t)} |\psi_0(x, t)\rangle \\
&= e^{-\frac{i}{\hbar} \int_0^t dt' E_0(t')} |\psi_0(x, t)\rangle
\end{aligned} \tag{6}$$

Another state contribution (with 1st order δt) is:

$$\begin{aligned}
U_1(t, 0) |\Psi(x, 0)\rangle &= -|\psi_2(x, t)\rangle \lim_{N \rightarrow \infty} \delta t \sum_{k=0}^N \Phi_{20}(k\delta t) e^{-\frac{it}{\hbar} \frac{k}{N} \frac{1}{k} \sum_{n_1=0}^k E_0(\frac{n_1}{N}t)} e^{-\frac{it}{\hbar} \frac{N-k}{N} \frac{1}{N-k} \sum_{n_2=k}^N E_2(\frac{n_2}{N}t)} \\
&= -|\psi_2(x, t)\rangle \lim_{N \rightarrow \infty} \delta t \sum_{k=0}^N \Phi_{20}(k\delta t) e^{-\frac{i}{\hbar} \frac{k}{N} \frac{1}{k} \int_0^{\frac{k}{N}t} dt' E_0(t')} e^{-\frac{i}{\hbar} (1-\frac{k}{N}) \frac{1}{1-\frac{k}{N}} \int_{\frac{k}{N}t}^t dt' E_2(t')} \\
&= -|\psi_2(x, t)\rangle t \int_0^1 dq \Phi_{20}(qt) e^{-\frac{i}{\hbar} \int_0^{qt} dt' E_0(t')} e^{-\frac{i}{\hbar} \int_{qt}^t dt' E_2(t')}
\end{aligned} \tag{7}$$

Another state contribution (with 2nd order δt) is:

$$\begin{aligned}
U_2(t, 0) |\Psi(x, 0)\rangle &= |\psi_0(x, t)\rangle t^2 \int_0^1 dq \int_0^q dq_1 \Phi_{20}(q_1 t) \Phi_{02}(qt) \\
&\quad e^{-\frac{i}{\hbar} \int_0^{q_1 t} dt' E_0(t')} e^{-\frac{i}{\hbar} \int_{q_1 t}^{qt} dt' E_2(t')} e^{-\frac{i}{\hbar} \int_{qt}^t dt' E_0(t')} \\
&\quad + |\psi_4(x, t)\rangle t^2 \int_0^1 dq \int_0^q dq_1 \Phi_{20}(q_1 t) \Phi_{42}(qt) \\
&\quad e^{-\frac{i}{\hbar} \int_0^{q_1 t} dt' E_0(t')} e^{-\frac{i}{\hbar} \int_{q_1 t}^{qt} dt' E_2(t')} e^{-\frac{i}{\hbar} \int_{qt}^t dt' E_4(t')}
\end{aligned} \tag{8}$$

which is starting to look strikingly like the Dyson series formulation. The exact time evolving coefficient for the ground state is written in terms of a pathway sequence $p_n(z)$ that ends on state $z = 0$:

$$\begin{aligned}
c_0(t) &= \lim_{N \rightarrow \infty} \sum_{n \text{ even}}^N t^n \prod_{j=1}^n \left(\int_0^{q_{n-j+1}} dq_{n-j} \Phi_{\{p_{n-1}(2), 0\}}(q_{n-j}t) e^{-\frac{i}{\hbar} \int_{q_{n-j}t}^{q_{n-j+1}t} dt' E_{\{p_{n-1}(2), 0\}}(t')} \right) \\
&\quad e^{-\frac{i}{\hbar} \int_0^{q_0 t} dt' E_0(t')} e^{\frac{i}{\hbar} \int_0^t dt' E_0(t')}
\end{aligned} \tag{9}$$

where $p_n(0) = \{p_{n-1}(2), 0\}$, $q_n = 1$. The n th term of the product goes to the right of the $(n-1)$ th term of the product. The ideal strategy would be to compute the $c_0(t)$, then use it in the time dependent probability amplitude coupled ODEs to solve for the time evolution of the other probability amplitudes. We can then test the condition that $\sum_{q=0}^{\infty} |c_q|^2 = 1$ at all times. Now, we shall make a simplification to test this formula - let $\omega(t) = \frac{1}{1+t}$. More on this strategy later. This leads to the simplification:

$$e^{-\frac{i}{\hbar} \int_{q_{n-j}t}^{q_{n-j+1}t} dt' (\frac{\hbar}{1+t} (b_{nkj} + \frac{1}{2}))} = \left(\frac{1 + q_{n-j}t}{1 + q_{n-j+1}t} \right)^{i(b_{nkj} + \frac{1}{2})}$$

where we have that $b_{nkj} - b_{nk(j-1)} = \pm 2$ depending on whether the particular sequence denoted by k goes up or down two states for the j th product term.

$$c_0(t) = \lim_{N \rightarrow \infty} \sum_{n_{\text{even}}}^N \left(\frac{t}{4}\right)^n (1+t)^{\frac{i}{2}} \sum_{k=1}^{C_{\frac{n}{2}}} a_{nk} \frac{\prod_{j=1}^n \left(\int_0^{q_{n-j+1}} d(q_{n-j}) \frac{(1+q_{n-j}t)^{(ib_{nkj} + \frac{i}{2})-1}}{(1+q_{n-j+1}t)^{(ib_{nkj} + \frac{i}{2})}} \right)}{(1+q_0t)^{\frac{i}{2}}} \quad (10)$$

We could continue here, but one of the problems that comes up is that specific sequences of states which alternate between 0th ground state and higher states will produce terms in the integrals that have power -1 (for the ground state energy, the quantum number $n = 0$), meaning that we attain logarithmic behaviour as well power behaviour arising naturally from the computation. We won't bother to continue here, other than to say that this formula for a small enough timestep would directly compute the time-evolution of the ground state of the 1D QHO problem with time dependent frequency (of course, given that I have not computationally tested this formula, I will reserve absolute judgement on its correctness). In the formula above, the sum in k corresponds to the permutation sequences that consist of consecutive even numbers that start with 0, end with 0, and have $n + 1$ elements. In this way, $C_{\frac{n}{2}}$ is the Catalan number, and $C_0 = 1$, $C_1 = 1$, $C_2 = 2$, and $C_3 = 5$, which corresponds to the number of pathway sequences by which the infinite product starts with the ground state and ends with the ground state after some time t . In general, $C_{\frac{n}{2}} = \frac{1}{\frac{n}{2}+1} \binom{n}{\frac{n}{2}}$. These pathways that determine the sequences of terms, they can be computed in code and truncate the series at some high order. a_{nk} corresponds to the term $\pm \sqrt{(n+1)_2}$ from the product Φ_{mn} functions associated with the k th state transition sequence that starts and ends with 0 (the ground state) with n state transitions. b_{nkj} is the quantum number associated with the j th state in the k th state sequence for n state transitions.

To this point, we've seen a relatively gruesome computational problem that seems to resist mathematical solution through brute force. However, AI found a far more elegant way to develop the solution from the time-dependent Schrodinger Equation. I will outline here mostly as an insight to how efficient the analysis of differential equations can be in finding solutions to problems in physics. Consider first the ansatz to the time evolution of the state vector that starts in the ground state of the 1D QHO problem. It is true that at all times, the Hamiltonian is even - this means that if the state vector begins in the even (Gaussian) ground state, the time-evolved solution will remain even. In fact, we assume that the time-evolved solution keeps the following form:

$$\Psi(x, t) = e^{A(t)x^2 + C(t)} \quad (11)$$

If this ansatz is true, it must satisfy the TDSE applied with the system starting in the ground eigenstate. To start, this implies:

$$\begin{aligned} i\hbar \frac{\partial \Psi(x, t)}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + \frac{1}{2} m \omega^2(t) x^2 \\ \implies i\hbar \Psi(x, t) \left(\dot{A}(t) x^2 + \dot{C}(t) \right) &= -\frac{\hbar^2}{2m} \Psi(x, t) (2A(t) + 4A^2(t) x^2) + \frac{1}{2} m \omega^2(t) x^2 \Psi(x, t) \quad (12) \\ \implies \dot{A}(t) &= \frac{2i\hbar}{m} A^2(t) + \frac{1}{2} \frac{m}{i\hbar} \omega^2(t) \text{ and } \dot{C}(t) = \frac{i\hbar}{m} A(t) \end{aligned}$$

The equation for $A(t)$ is a Ricatti equation. To linearize it, we introduce a real factor $\rho(t)$ to specify $A(t)$:

$$A(t) = -\frac{m}{2\hbar\rho^2(t)} + i\frac{m\dot{\rho}(t)}{2\hbar\rho(t)}$$

$$\dot{A}(t) = \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)} + i\frac{m\ddot{\rho}(t)}{2\hbar\rho(t)} - i\frac{m\dot{\rho}^2(t)}{2\hbar\rho^2(t)}$$

Substituting $A(t)$ back into Equation 12, we get:

$$\begin{aligned} \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)} + i\frac{m\ddot{\rho}(t)}{2\hbar\rho(t)} - i\frac{m\dot{\rho}^2(t)}{2\hbar\rho^2(t)} &= \frac{2i\hbar}{m} \left(-\frac{m}{2\hbar\rho^2(t)} + i\frac{m\dot{\rho}(t)}{2\hbar\rho(t)} \right)^2 + \frac{1}{2} \frac{m}{i\hbar} \omega^2(t) \\ \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)} + i\frac{m\ddot{\rho}(t)}{2\hbar\rho(t)} - i\frac{m\dot{\rho}^2(t)}{2\hbar\rho^2(t)} &= \frac{2i\hbar}{m} \left(\frac{m^2}{4\hbar^2\rho^4(t)} - \frac{m^2\dot{\rho}^2(t)}{4\hbar^2\rho^2(t)} - i\frac{m^2\dot{\rho}(t)}{2\hbar^2\rho^3(t)} \right) - i\frac{1}{2} \frac{m}{\hbar} \omega^2(t) \\ \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)} + i\frac{m\ddot{\rho}(t)}{2\hbar\rho(t)} - i\frac{m\dot{\rho}^2(t)}{2\hbar\rho^2(t)} &= \left(i\frac{m}{2\hbar\rho^4(t)} - i\frac{m\dot{\rho}^2(t)}{2\hbar\rho^2(t)} + \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)} \right) - i\frac{1}{2} \frac{m}{\hbar} \omega^2(t) \\ \implies \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)} &= \frac{m\dot{\rho}(t)}{\hbar\rho^3(t)}, \text{ trivially, and} \\ \implies \frac{m\ddot{\rho}(t)}{2\hbar\rho(t)} &= i\frac{m}{2\hbar\rho^4(t)} - \frac{1}{2} \frac{m}{\hbar} \omega^2(t) \implies \ddot{\rho}(t) + \omega^2(t)\rho(t) = \frac{1}{\rho^3(t)} \end{aligned} \quad (13)$$

Where this last equation is known as the Ermakov-Pinney ODE, which has a unique solution that defines the parameter $\rho(t)$. Thus, the specified $A(t)$ and $C(t)$ (once solved for) solve the TDSE. Some sources will give the scaled Ermakov-Pinney ODE (where $\rho \rightarrow \sqrt{m}\rho$):

$$\ddot{\rho}(t) + \omega^2(t)\rho(t) = \frac{1}{m^2\rho^3(t)}$$

Regardless, the proposed definition for $A(t)$ can be used to solve for $C(t)$ in terms of $\rho(t)$:

$$\begin{aligned} \dot{C}(t) &= -\frac{i}{2\rho^2(t)} - \frac{\dot{\rho}(t)}{2\rho(t)} \\ \implies C(t) &= C(0) - \frac{i}{2} \int_0^t dt' \frac{1}{\rho^2(t')} - \frac{1}{2} \ln \left(\frac{\rho(t)}{\rho(0)} \right) \\ \implies e^{C(t)} &= e^{C(0) - \frac{i}{2} \int_0^t dt' \frac{1}{\rho^2(t')}} \sqrt{\frac{\rho(0)}{\rho(t)}} \end{aligned} \quad (14)$$

With normalization, we can solve for $e^{C(0)}\sqrt{\rho(0)} = \left(\frac{m}{\pi\hbar}\right)^{\frac{1}{4}}$ given that $\Psi(x, 0) = |\psi_n(x, 0)\rangle$. Then, we can substitute back to solve for $\Psi(x, t)$:

$$\Psi(x, t) = \left(\frac{m}{\pi\hbar\rho^2(t)} \right)^{\frac{1}{4}} e^{-\frac{mx^2}{2\hbar\rho^2(t)} + i\frac{m\dot{\rho}(t)x^2}{2\hbar\rho(t)} - \frac{i}{2} \int_0^t dt' \frac{1}{\rho^2(t')}} \quad (15)$$

where, evidently, $\rho(0) = \frac{1}{\sqrt{\omega(0)}}$ and $\dot{\rho}(0) = 0$ for the initial condition. As an implication of the Ermakov-Pinney ODE, we find:

$$\ddot{\rho}(0) = 0$$

Now, we can solve easily for the time-dependent probability amplitudes:

$$\begin{aligned} c_n(t) &= \langle \psi_n(x, t) | \Psi(x, t) \rangle e^{\frac{i}{\hbar} \int_0^t dt' E_n(t')} \\ \implies c_0(t) &= \sqrt{\frac{2\sqrt{\frac{\omega(t)}{\rho^2(t)}}}{\omega(t) + \frac{1}{\rho^2(t)} - i\frac{\dot{\rho}(t)}{\rho(t)}}} e^{-\frac{i}{2} \int_0^t dt' \frac{1}{\rho^2(t')} + \frac{i}{2} \int_0^t dt' \omega(t')} \end{aligned} \quad (16)$$

One could consider the special exception of $\omega(t) = \frac{1}{\rho^2(t)}$, which would lead to substantial simplification. This concludes this blog post.